

Néel and Valence-Bond Crystal phases of the Two-Dimensional Heisenberg Model on the Checkerboard Lattice

S. Moukouri

*Department of Physics and Michigan Center for Theoretical Physics
University of Michigan 2477 Randall Laboratory, Ann Arbor MI 48109*

I use an improved version of the two-step density matrix renormalization group method to study ground-state properties of the 2D Heisenberg model on the checkerboard lattice. In this version the Hamiltonian is projected on a tensor product of two-leg ladders instead of chains. This allows investigations of 2D isotropic models. I show that this method can describe both the magnetically disordered and ordered phases. The ground-state phases of the checkerboard model as J_2 increases are: (i) Néel with $Q = (\pi, \pi)$, (ii) a valence bond crystal (VBC) of plaquettes, (iii) Néel with $Q = (\pi/2, \pi)$, and (iv) a VBC of crossed dimers. In agreement with previous results, I find that at the isotropic point $J_2 = J_1$, the ground state is made of weakly interacting plaquettes with a large gap $\Delta \approx 0.67J_1$ to triplet excitations.

Frustration-induced magnetically disordered phases in two dimensions (2D) recently have attracted substantial interest [1]. Frustrated magnets are known to display unconventional ground states with, in some cases, a large set of low-lying degenerate singlet excitations that are still not well understood. Among models of frustrated systems, the Heisenberg model on the checkerboard lattice (HMCL) has recently been intensively studied by various techniques [2, 3, 4, 5, 6, 7]. This model is seen as a first step in the investigation of the 3D pyrochlore model. The emerging picture is that at the isotropic point ($J_1 = J_2$), the HMCL spontaneously breaks the lattice's translational symmetry. The ground state is a singlet made of a collection of weakly coupled plaquettes with a large gap, $\Delta \approx 0.7J_1$, to triplet excitations. Away from the isotropic point, the situation is less clear. There is no single method which can capture the full phase diagram.

In this letter, I introduce an improved version of the two-step density-matrix renormalization group (TSDMRG) [8, 9] which, as I will show, is very convenient in the study of the HMCL and other 2D frustrated models. This new version is based on using the two-leg ladder, instead of chains, as the starting point to build the 2D lattice. The main insight in using the two-leg ladder to construct the 2D lattice comes from large N predictions [11] that frustration often induces ground states in which the translational symmetry is broken. In the strong-coupling regime of the disordered phase of $S = 1/2$ systems, the system is made of a collection of singlets or plaquettes. This strong coupling regime cannot be described starting from independent chains which are gapless. Starting from a single chain, small transverse perturbations can yield a gap within the TSDMRG. But this gap is often small and it is difficult to obtain reliable extrapolations. The two-leg ladder does not present this problem. It does already present a large gap $\Delta \approx 0.5$ even in absence of frustration. Coupled ladders naturally evolve toward the 2D Néel state as the number of legs increases. Hence, in principle, disordered and or-

dered phases could be described within a two-leg ladder version of the TSDMRG. This suggests that the two-leg ladder is a more natural starting point to describe ground state phases of 2D antiferromagnets than the single chain.

Additional insights into this idea came from my comparative study of coupled chains with half-integer and integer spins [10]. In Ref.[10], when starting from single chains, I found that although chains with $S = 1$ display the Haldane gap, $\Delta \approx 0.4$, they converge much faster to the Néel state than those with $S = 1/2$. Furthermore, when a frustration induced disordered phase is present, it can be much more easily found in the case $S = 1$. Hence, following the equivalence between the two-leg ladder and the Haldane spin chain, suggested by the Affleck-Kennedy-Lieb-Tasaki construction [12], it would be better to adopt the two-leg ladder as the building block for two-dimensional lattices.

I will now illustrate this idea in the case of the HMCL. Following the usual notation, the HMCL is given by:

$$H = J_1 \sum_{\langle i,j \rangle} \mathbf{S}_i \mathbf{S}_j + J_2 \sum_{[i,j]} \mathbf{S}_i \mathbf{S}_j, \quad (1)$$

where $\langle i, j \rangle$ represents nearest-neighbor sites and $[i, j]$ stand for next-nearest neighbors on every other plaquette. J_1 is set as the unit energy.

The TSDMRG with ladders is similar to the method with chains. So I refer the reader to Ref.[8, 9] for a complete exposition of the algorithm. Here, I will discuss only briefly the main points of the algorithm. I start by dividing the 2D lattice into two-leg ladders; the Hamiltonian (1) is written as,

$$H = \sum_{\text{ladders}} H_{\text{ladder}} + H_{\text{int}}, \quad (2)$$

where H_{ladder} is the Hamiltonian of a single two-leg ladder, H_{int} contains the inter-ladder part. In the first step of the method, the usual DMRG method is applied to

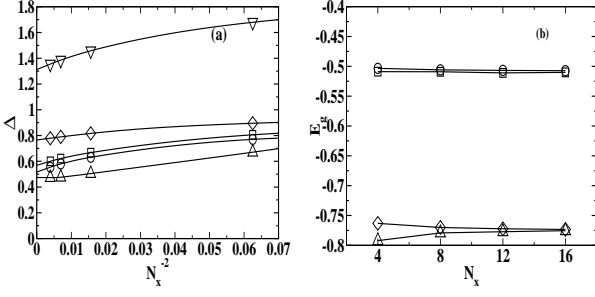


FIG. 1: (a) Spin gap of the two-leg ladder for $J_2 = 0$ (circles), 0.5 (squares), 1 (diamonds), 1.1 (triangles up), and 2 (triangles down). (b) Ground-state energies as function of the system size for a two-leg ladder for $J_2 = 1$ (circles), $J_2 = 2$ (diamonds), and for the 2D lattice for $J_2 = 1$ (squares), $J_2 = 2$ (triangle up).

generate a low energy Hamiltonian of an isolated ladder of N_x sites keeping m_1 states. Then m_2 low-lying states of the superblock states, the corresponding energies, and all the local spin operators are kept. These energies represent the renormalized low energy Hamiltonian of a single ladder. The Hamiltonian (2) is then projected onto the tensor product basis of independent ladders,

$$\Psi = \prod_{\text{ladders}} \Phi_{\text{ladder}}, \quad (3)$$

where Φ_{ladder} is an eigenfunction of $H_{0,\text{ladder}}$. This yield an effective Hamiltonian,

$$H_{\text{eff}} = \sum_{\text{ladders}} H_{0,\text{ladder}} + \tilde{H}_{\text{int}}. \quad (4)$$

The resulting effective coupled ladder problem which is 1D is studied again by the DMRG method in the transverse direction. The TSDMRG is variational, as the original DMRG method, the subspace spanned by the wavefunctions of the form Ψ is a subspace of the full Hilbert space of Hamiltonian (1). Its convergence depends on m_1 and m_2 , the error is given by $\max(\rho_1, \rho_2)$, where ρ_1 and ρ_2 are the truncation errors in the first and second steps respectively. m_2 fixes the energy band-width δE . The method is accurate only when the inter-ladder couplings are small with respect to δE . In the present simulations $\delta E \approx 4$. Since for the HMCL the inter-ladder and intra-ladder are of the same magnitude, in principle this approach would be plagued by the same deficiencies the block RG method. But if the starting point is chosen so that the essential physics is already contained at the level of the ladder, the effective strength of the inter-ladder couplings will be small even if the bare couplings

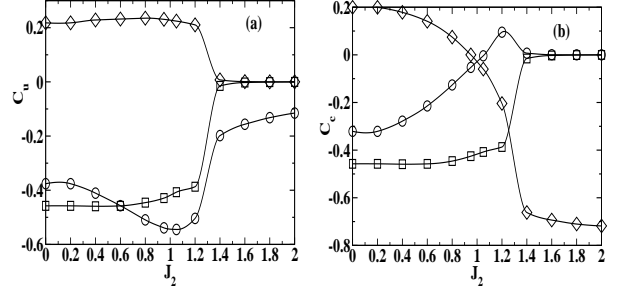


FIG. 2: Short-range correlations C_l (circles), C_r (squares), C_d (diamonds) for the two-leg ladder for uncrossed (a) and crossed (b) plaquettes as function of J_2

are not. This is particularly the case of models with frustration in which the competing interactions largely cancel each other in the strong frustration regime, yielding weakly coupled sub-clusters.

The ground state properties of an isolated ladder can readily be obtained. I keep up to $m_1 = 96$ and $N_x = 16$ and I target spin sectors from $S_z = 0$ to $S_z = \pm 4$ and used open boundary conditions (OBC). The maximum error is $\rho_1 = 1 \times 10^{-4}$. There is a gap Δ for all values of J_2 investigated between 0 and 2. The finite size behavior of gaps for some typical values of J_2 are shown in Fig.1. The case $J_2 = 0$ reduces to the usual two-leg ladder which has been widely studied in the literature [13]. For $J_2 = 0$, $\Delta \approx 0.5$. As J_2 increases, Δ has a non-monotonous behavior. This suggests a rich structure which is revealed more clearly by the analysis of the correlation functions. I computed the following short-range correlation functions: the bond strength along a leg $C_{l_{u,c}} = \langle \mathbf{S}_{i,1} \mathbf{S}_{i+1,1} \rangle_{u,c}$ for uncrossed (u) and crossed (c) plaquettes, the diagonal correlation $C_{d_{u,c}} = \langle \mathbf{S}_{i,1} \mathbf{S}_{i+1,2} \rangle_{u,c}$, and bond strength along the rungs $C_r = \langle \mathbf{S}_{i,1} \mathbf{S}_{i,2} \rangle$. Note that I have introduced a second index to the local spin. These correlations are shown in Fig.2. Four regions can be identified: (i) region I (rung dimers): $0 \lesssim J_2 \lesssim 0.6$, $C_{l_{u,c}} < 0$, $C_{l_u} \approx C_{l_c}$, $C_{d_{u,c}} > 0$, $C_r < 0$, and $|C_r| > |C_{l_u}|$; the dominant spin-spin correlations are along the rungs. The ground state properties of the ladder in this region are identical to those of the unfrustrated ladder ($J_2 = 0$). (ii) Region II (plaquettes I): $0.6 \lesssim J_2 \lesssim 1$, $C_{l_{u,c}} < 0$, $|C_{l_u}| > |C_{l_c}|$, $C_{d_{u,c}} > 0$, $C_r < 0$, and $|C_r| < |C_{l_u}|$; the physics is dominated by that of the isotropic point. At this point, the ground state is a collection of weakly interacting uncrossed plaquettes. Both C_{d_c} and C_{l_c} vanish at $J_2 = 1$. In this region, the local spin configuration is the same on all the uncrossed plaquettes as shown in Fig.3(b). (iii) region III (plaquettes II): $1 \lesssim J_2 \lesssim 1.3$, $C_{l_u} < 0$, $C_{l_c} > 0$, $C_{d_{u,c}} > 0$, $C_{d_c} < 0$, $C_r < 0$, and $|C_r| < |C_{l_u}|$; in this region, the ground state is again dominated by uncrossed plaquettes. But now the local spin configura-

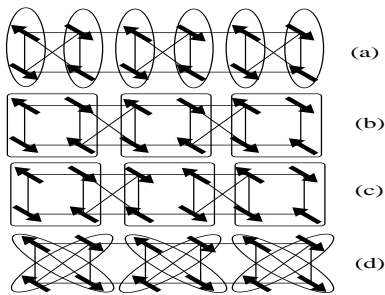


FIG. 3: The four phases of the two-leg ladder: rung dimers (a), plaquette I (b), plaquette II (c), and crossed dimers (d).

tions on two consecutive uncrossed plaquettes are images of one another by reflection with respect to a plane passing through the middle of the crossed plaquette between them. Region IV (crossed dimers): $1.3 \lesssim J_2$, $C_{l_u} < 0$, $C_{d_c} < 0$, $C_{l_c} = C_r = C_{d_u} \approx 0$, and $|C_r| < |C_{l_u}|$; the ground state is dominated by the crossed dimers on crossed plaquettes as shown in Fig.3(d). The sketch of the spin structure corresponding to each region is summarized in Fig.3. Since I applied OBC, for a given size, there are two possible ground states depending on the plaquette pattern: **(a)** *ucu...ucu* or **(b)** *cuc...cuc*. In region I, the configurations **(a)** and **(b)** have nearly the same energy. This is consistent with the fact that the translational symmetry is not broken. But in Region II and III, **(a)** has the lowest energy, since it has a larger number of uncrossed plaquettes. By contrast, in Region IV where dimer order is dominant, it is **(b)** that has the lowest energy.

The 2D systems are obtained by applying the DMRG on H_{eff} in the transverse direction. I studied systems of size $N_x \times N_y = 4 \times 6$, 8×10 , 12×14 and 16×18 . I kept up to $m_2 = 96$ and used OBC. Inter-ladder interactions will have very different effects depending on whether they correspond to a magnetic regime or a disordered regime. I will first consider their effects on region II, which includes the isotropic point. Recently, there have been a number of studies which strongly suggest that the physics of the 2D systems is identical to that displayed by the two-leg ladder. In other words, the ground state is essentially made of weakly interacting plaquettes. If this is the case, it means that the inter-ladder interactions will not strongly modify the ground state wave function of decoupled ladders. Fig.1 shows that the ground state energy and Δ remain very close to that of an isolated plaquette. Thus in the vicinity of $J_2 = 1$, inter-ladder interactions do not strongly renormalize the properties of an isolated ladder which themselves are close to those of an isolated plaquette. The extrapolated gap is found to be $\Delta = 0.67J_1$ which is in good agreement with the prediction from exact diagonalization [5]. The same conclusion is seen in Fig.1 for region IV where the crossed-

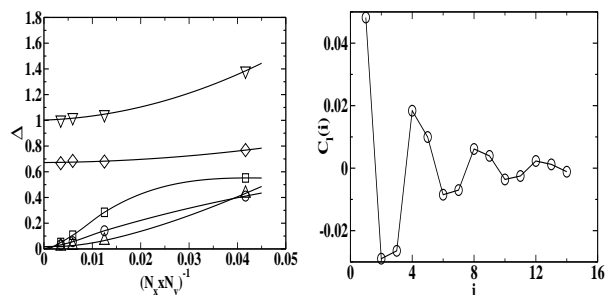


FIG. 4: (a) 2D gaps as function of the system size $J_2 = 0$ (circles), 0.5 (squares), 1 (diamonds), 1.1 (triangles up), and 2 (triangles down). (b) Correlation function along the legs as function of the distance for $J_2 = 1.25$.

dimer ground state found for the ladder is also the ground state of the 2D lattice. In both cases, the wave function made of the tensor product of the wave function of single two-leg ladders is a good variational wave function for the 2D system. In each case, the ground state energy of the 2D system remains very close to that of individual plaquettes or crossed dimers. This can be explained as follows: when ladders are brought together to build the 2D lattice, the dominant local correlations are C_{l_u} in region II and C_{d_c} in region IV; during this process, magnetic energy cannot efficiently be gained. For region II, this is because the two neighboring plaquettes of an uncrossed plaquette in the direction of the rungs involve frustrated bonds. Hence the system prefers the original configuration to avoid increasing its energy. For region IV, C_r is very small. The system cannot increase it when the ladders are coupled, because the spins are already involved in strong diagonal dimers. There is, however, the possibility to gain magnetic energy by forming Néel order along the direction of the diagonal bonds (J_2 direction) as suggested in Ref.[7]. This is unlikely, however, because once such a phase is reached, I do not see how the system could go to crossed dimers at larger J_2 . The action of J_1 which act as frustration in this regime decreases as J_2 increases. Hence once this hypothetical Néel phase along the J_2 bonds is reached, there is no obvious mechanism that could destroy it as J_2 increases to yield the crossed-dimer phase as suggested in Ref.[7]. Such a Néel phase would be favored only when $J_2 \gg J_1$. I made rough calculations with $J_2 = 4, 8$ and I found that the system remains in the crossed-dimer phase. The situation is apparently identical to the $J_1 - J_2$ chain where the independent chains regime is only reached in the infinite J_2 limit.

The situation is very different for regions I and III. In region I, the dominant local correlation is C_r ; when the ladders are brought together, magnetic energy can be gained by an antiferromagnetic arrangement along the

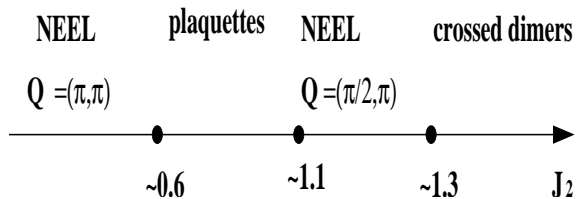


FIG. 5: Ground-state phases of the 2D checkerboard model as function of J_2 . Note that the phase boundaries are rough estimates taken from the phases of the two-leg ladder.

rungs. This enhances the local antiferromagnetic order which exists along the legs and ultimately leads to a Néel order with $Q = (\pi, \pi)$. This is seen in the vanishing of the spin gap for $J_2 = 0$ and $J_2 = 0.5$ shown in Fig.4(a). This is in agreement with results for $J_2 = 0$ from quantum Monte Carlo (QMC) simulations [14] and large S analysis [4]. I find that the TSDMRG ground state energy -0.6011 at $J_2 = 0$, is not in very good agreement with the QMC result -0.6699 of Ref.[14]. Despite this discrepancy, the TSDMRG is nevertheless able to reproduce the low-energy behavior of the ordered phase. This is not in fact surprising. In the Resonating valence bond picture, the Néel state and its low energy excitations can be written as linear combination of a tensor product of dimers. The TSDMRG variational solution of Hamiltonian(1) which is a linear combination of the wave functions Ψ has exactly this form. A similar analysis also applies for region III. C_{l_u} is dominant in region II. But as seen in Fig.2, C_{l_u} has a minimum at $J_2 = 1$ and then increases. It becomes very close to C_r when J_2 enters region III. Hence magnetic energy can be gained again through the rungs. Since the structure along the legs is not modified from Fig.3(d), the resulting wave vector will be $Q = (\pi/2, \pi)$. This is seen in Fig.4 in the behavior of the spin-spin correlation function $C_l(i)$ along the legs. $C_l(i)$ displays a period of 4. The correlations between the rungs (not shown) oscillate with $q_y = \pi$. Fig.5 presents a sketch of the different ground state phases of the HMCL as function of J_2 . I note that in Ref.[7], a very similar phase diagram was suggested; the only difference with the TSDMRG phase diagram is the wave vector of the Néel phase between the plaquette and crossed-dimer phases.

In summary, I have shown that the TSDMRG method can reliably be used to study the disordered phases with

short correlation lengths of isotropic 2D models. In these phases, the system is a collection of dimers or plaquettes. This makes the two-leg ladder a very good starting point for a variational calculation. I showed that the basic physics of 2D systems could already be read through short-range correlations of the two-leg ladders. This variational calculation is able to predict reasonably magnetically ordered phases as well. In this work, I did not discuss the question of low-lying singlet excitations within the gap. Targeting them will lead to large truncation errors and the calculations will become impractical. These excitations are naturally truncated out when they are not needed to form a target state. Finally, The same method could be applied to the Sutherland-Shastry, $J_1 - J_2$ or the Kagomé models in 2D. It could also be applied to the pyrochlore lattice, provided that the Hamiltonian could be written in some form involving 1D subsystems with a large gap.

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